Imbalanced Fermi superfluid in a one-dimensional optical potential

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Abstract

The superfluid properties of a two-state Fermi mixture in an optical lattice are profoundly modified when an imbalance in the population of the two states is present.We present analytical solutions for the free energy, and for the gap and number equations in the saddle-point approximation describing resonant superfluidity in the quasi-two-dimensional gas. Inhomogeneities due to the trapping potentials can be taken into account using the local density approximation. Analyzing the free energy in this approximation, we find that phase separation occurs in the layers. The phase diagram of the superfluid and normal phases is derived and analytical expressions for the phase lines are presented. We complete the investigation by accounting for effects beyond mean-field in the BEC limit where the system is more properly described as a Bose-Fermi mixture of atoms and molecules.

The formation of pairing correlations in a mixture of two types of fermions is frustrated when the number of fermions in each state is unequal. The effect of such "spin imbalance" on pairing has been investigated theoretically since Clogston's seminal work [1] for conventional superconductors, and has led to the prediction of novel pairing states [2], i.a. relevant for color superconductivity in dense quark matter [3] and for neutron-proton pairing in asymmetric nuclear matter [4]. The experimental study of Fermi superfluids with imbalanced spin population has only recently become possible, in ultracold atomic gases [5, 6], renewing theoretical interest in imbalanced superfluidity [7, 8, 9].

In these experiments, the interaction strength between ultracold fermions can be precisely controlled through the use of Feshbach resonances. These scattering resonances allow to tune the s-wave scattering length from a large negative value, giving rise to a Bardeen-Cooper-Schrieffer (BCS) superfluid [10], to a large positive value where a Bose-Einstein condensate (BEC) of weakly bound molecules is formed [11].

Also the trapping geometry confining the Fermi gas can be precisely controlled experimentally. Of particular interest is the possibility to impose a crystalline potential through the use of optical lattices. These allow to experimentally mimic theoretical lattice models such as the Hubbard model. One-dimensional optical lattices allow to study stacked layers of superfluid and create a geometry analogous to layered (cuprate) high-temperature superconductors. Optical lattices have been used to demonstrate superfluid behavior of condensates [12], and to probe the Mott-superfluid transition [13]. So far, fermionic superfluidity in an optical lattice has only been studied [14] with balanced Fermi gases.

We investigate the effect of spin imbalance on the superfluid properties of a Fermi gas in an optical lattice. In particular, we will examine the case of a one-dimensional optical lattice generated by two counterpropagating laser beams (parallel to the z-axis) with wave length λ. These laser beams generate a periodic potential $V_0 \sin^2 (2\pi z/\lambda)$. When loaded in this optical lattice, the gas forms a stack of typically a few hundred quasi-2D layers containing several thousands of atoms each. The interaction between atoms within a given quasi-2D layer can be modelled by a 2D contact interaction whose strength g depends on the model cutoff K_c and on the energy of the scattering atoms through [15]

$$\frac{1}{g} = \frac{m}{4\hbar^2} \left[i - \frac{\ln (E/E_b)}{\pi} \right] - \int_{k<K_c} \frac{d^2\mathbf{k}}{(2\pi)^3} \frac{1}{(\hbar k)^2/m - E + i\varepsilon}. \tag{1}$$

Here, m is the mass of the atoms and E_b is the energy of the bound state that always exists

in two dimensions, given by

$$E_b = \frac{C\hbar\omega_L}{\pi} \exp\left(\sqrt{2\pi}\frac{\ell_L}{a_s}\right), \tag{2}$$

with a_s the (3D) s-wave scattering length of the fermionic atoms, $\omega_L = \sqrt{8\pi^2 V_0/(m\lambda^2)}$ and $\ell_L = \sqrt{\hbar/(m\omega_L)}$ and $C \approx 0.915$ (cf. Ref. [16]).

In this letter we derive an *analytical* expression for the free energy of the gas with density n in a layer in the optical potential. Extremizing this free energy with respect to the superfluid gap allows to set up and solve the gap equation. We derive analytical expression for both the gap and the chemical potential, for fixed imbalance. However, we will argue that the imbalanced gas may be unstable with respect to phase separation into a balanced superfluid and a halo of excess carriers, similar to the three-dimensional case [8], and we derive the phase diagram for the gas, again retrieving analytic expressions for the phase boundaries.

The partition sum of the quasi-2D Fermi gas can be written as a path integral over the exponential of the action functional S for the fermionic fields $\bar{\psi}_{k,\sigma}, \psi_{k,\sigma}$ where σ denotes the spin. We write $k = \{\mathbf{k}, \omega_n\}$ for the 2D wave number $\mathbf{k}$ and the Matsubara frequency $\omega_n = (2n+1)\pi/\beta$ where $\beta = 1/(k_B T)$ is the inverse temperature:

$$\mathcal{Z} = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \exp\{-\mathcal{S}\}, \tag{3}$$

with

$$\mathcal{S} = \frac{1}{\beta}\sum_{\omega_n}\int_\mathcal{B}\frac{d\mathbf{k}}{(2\pi)^2}\left\{\sum_{\sigma=\uparrow,\downarrow}\bar{\psi}_{k,\sigma}\left[-i\omega_n + \mathbf{k}^2 - \mu_\sigma\right]\psi_{k,\sigma} + g\bar{\psi}_{k,\uparrow}\bar{\psi}_{-k,\downarrow}\psi_{-k,\downarrow}\psi_{k,\uparrow}\right\}. \tag{4}$$

Here, we use units such that $\hbar = k_F = E_F = 1$. The number of spin-up and spin-down fermions is controlled through the chemical potentials $\mu_\uparrow$ and $\mu_\downarrow$. The partition sum corresponding to the action functional (4) can be calculated following the standard procedure of introducing the Hubbard-Stratonovic decomposition, integrating out the Grassman variables, and performing the saddle-point approximation [17, 18] with a constant gap Δ. We therefore neglect the possibility of two-dimensional FFLO type states with a modulated order parameter [2, 19]. It is useful to express the results as a function of $\mu = (\mu_\uparrow + \mu_\downarrow)/2$ determining the total number of fermions and $\zeta = (\mu_\uparrow - \mu_\downarrow)/2$ expressing the imbalance in chemical potentials. We find $\mathcal{Z}_{sp} = \exp\{-\beta\Omega_{sp}\}$ with

$$\Omega_{sp} = -\frac{\Delta^2}{g} - \frac{1}{\beta}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\left\{\log\left[2\cosh(\beta\zeta) + 2\cosh(\beta E_k)\right] - \beta\xi_k\right\}. \tag{5}$$

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Here the k-integration is convergent at large wave vectors so that the wave vector cutoff K_c can be sent to infinity, Δ represents the pairing gap, $\xi_k = k^2 - \mu$ is the free particle spectrum, and $E_k = \sqrt{\xi_k^2 + \Delta^2}$ is the Bogoliubov spectrum. The saddle-point free energy Ω_{sp} allows to derive the gap and number equations. A similar result was derived for the homogeneous 3D gas by Iskin and Sa de Melo [9]. For the 2D case however, we succeeded to perform the wave-number integrations analytically in the limit of temperature going to zero:

$$
\begin{aligned}
8\pi\Omega_{sp} = {} & -\Delta^2 \ln\left(E_b\right) - \mu\left(\sqrt{\mu^2 + \Delta^2} + \mu\right) + \Delta^2 \ln\left(\sqrt{\mu^2 + \Delta^2} - \mu\right) - \frac{\Delta^2}{2} \\
& - 2\zeta\left(k_b^2 - k_a^2\right) + \xi_b\sqrt{\xi_b^2 + \Delta^2} - \xi_a\sqrt{\xi_a^2 + \Delta^2} + \Delta^2 \ln\left(\frac{\sqrt{\xi_b^2 + \Delta^2} + \xi_b}{\sqrt{\xi_a^2 + \Delta^2} + \xi_a}\right)
\end{aligned}
\tag{6}
$$

where $\xi_{a,b} = k_{a,b}^2 - \mu$ and for $\zeta > \sqrt{\Delta^2 + (\min[\mu,0])^2}$

$$
\begin{cases}
k_a = \sqrt{\max[\mu - \sqrt{\zeta^2 - \Delta^2}, 0]} \\
k_b = \sqrt{\mu + \sqrt{\zeta^2 - \Delta^2}}
\end{cases}
\tag{7}
$$

For $\zeta \leqslant \sqrt{\Delta^2 + (\min[\mu,0])^2}$ the terms containing k_a and k_b in (6) vanish. The Bogoliubov energy E_k for quasiparticle excitations with wave vector $k = k_a, k_b$ becomes equal to the imbalance of the chemical potentials ζ. All quasiparticle states with $k \in [k_a, k_b]$ have a Bogoliubov energy less than ζ, and contribute as normal state particles, rather than as superfluid excitations, to the free energy.

Iskin and Sa de Melo [9] solve the gap and number equations for the imbalanced three-dimensional superfluid numerically with respect to ζ, μ and Δ for a given imbalance $\delta n/n$ and a given interaction strength g. In the two-dimensional case, this procedure applied to (5), yields analytical results, summarized in Table I. However, the question can be raised as to whether the state with fixed $\delta n/n$ is stable with respect to phase separation into a phase with a balanced superfluid ($\delta n/n = 0$) in the center of the trap and an imbalanced halo of excess spin component surrounding it. Indeed, in the experiment of Ketterle and co-workers [20] for a three-dimensional gas with a nonuniform trapping potential, the excess spin component is expelled in a shell surrounding a spin-balanced superfluid . Will this be similar for a 2D gas within a layer of the optical potential ?

If we consider a 2D trapping potential $V(\mathbf{r})$ that varies slowly on the length scales set by the interparticle distance $\ell = n^{-1/2}$ and the superfluid gap $\ell_\Delta = \sqrt{\hbar^2/m\Delta}$, we can apply the

	$E_b/2 < (\delta n/n)^2 E_F$	$(\delta n/n)^2 E_F < E_b/2$
Δ^2	0	$2E_b E_F \left(1 - h\left(E_F/E_b\right)\dfrac{\delta n}{n}\right)$
μ	E_F	$E_F - \dfrac{E_b}{2}\left(1 - h\left(E_F/E_b\right)\dfrac{\delta n}{n}\right)$

TABLE I: Analytical solutions for Δ^2 and μ at fixed imbalance $\delta n/n$ and binding energy E_b, where $h(x) = \max\left[\sqrt{2x}, 1\right]$. For $E_b/(2E_F) < (\delta n/n)^2$ superfluidity is suppressed. There is a qualitative change in the dependence of Δ^2 and μ on E_b when E_b becomes equal to $2E_F$; this value can be intepreted as separating a 'weak coupling' from a 'strong coupling' regime.

procedure outlined by De Silva and Mueller [21] for the imbalanced gas in a regular three-dimensional trap. That is, we calculate $n(\mathbf{r})$ and $\delta n(\mathbf{r})$ in the local density approximation, where the local average chemical potential equals $\mu = \mu_0 - V(\mathbf{r})$ and the difference between the chemical potentials $\zeta = \zeta_0$ is constant in space for a spin-independent trapping potential:

$$n(\mathbf{r}) = -\left.\partial\Omega_{sp}/\partial\mu\right|_{\mu=\mu_0-V(r),\zeta=\zeta_0} \tag{8}$$

$$\delta n(\mathbf{r}) = -\left.\partial\Omega_{sp}/\partial\zeta\right|_{\mu=\mu_0-V(r),\zeta=\zeta_0}. \tag{9}$$

The gap is then found by extremizing Ω_{sp} with respect to Δ, for μ and ζ fixed by the local density approximation, rather than for $\delta n/n$ fixed. The validity of this procedure depends on whether the local density approximation is justified; this need not be the case for all experimental setups [6].

For $\zeta = 0$, we find that, the free energy Ω_{sp} shows a single minimum at $\Delta_{\mathrm{bal}} = \sqrt{2E_b(\mu + E_b/2)}$ [15], where its value is $\Omega_{\mathrm{bal}} = -(\mu + E_b/2)^2/(4\pi)$. This minimum represents the superfluid state (since $\Delta \neq 0$). As the imbalance ζ is increased, Ω_{sp} develops a second minimum around $\Delta = 0$, representing the normal state. The free energy of the normal state is $\Omega_0 = -[(\mu+\zeta)^2\Theta(\mu+\zeta > 0) + (\mu - \zeta)^2\Theta(\mu - \zeta > 0)]/(8\pi)$. We have verified numerically that no other minima of Ω_{sp} except the ones at $\Delta = \Delta_{\mathrm{bal}}$ and $\Delta = 0$ occur.

Upon increasing ζ the free energy curves are only affected in the region $\Delta < \zeta$. The minimum at $\Delta = \Delta_{\mathrm{bal}}$, representing the superfluid state, is therefore not affected by changes in ζ until it ceases to exist: Ω_{bal} is independent of ζ. From this it follows that the superfluid state does not sustain imbalance ($\delta n = 0$ since $\partial\Omega_{\mathrm{bal}}/\partial\zeta = 0$). The free energy of the normal state, Ω_0, does depend on ζ, so that the normal state supports imbalance, as expected. This scenario is similar to that for a 3D imbalanced Fermi mixture [8].
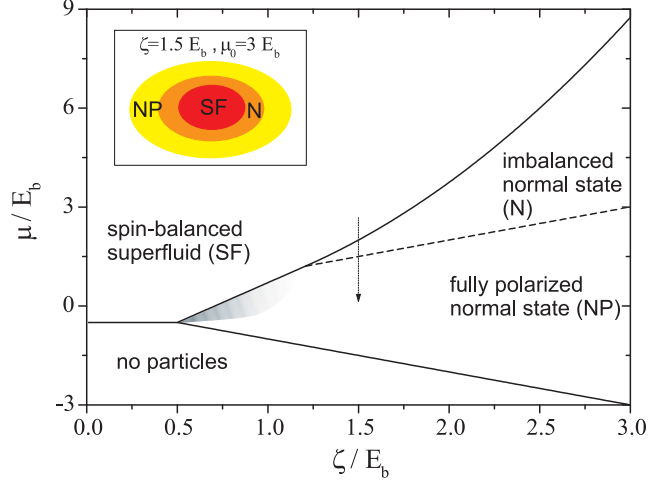
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FIG. 1: The phase diagram for the imbalanced (two-dimensional) Fermi gas is shown as a function of the average chemical potential μ and the difference between the chemical potentials ζ. Three phases can be identified: a balanced superfluid (SF), an imbalanced normal sate (N) and a fully polarized normal state (NP). The arrow indicates the path in the phase diagram that is traversed when moving away from the center of a 2D trap towards the edges. The corresponding overall shell structure is illustrated in the inset. At very strong coupling (large E_b) we expect corrections beyond mean field to push the phase line down into the shaded region, where also a mixture of bosonic molecules and fermionic atoms can appear.

To evaluate the phase boundary between the balanced superfluid and the imbalanced normal state, we should make a distinction between the cases $\mu > \zeta$ and $\mu < \zeta$. For $\mu > \zeta$ the thermodynamic potentials of the superfluid and normal state are equal for $\mu E_b = \zeta^2 - (E_b/2)^2$, whereas for $\zeta > \mu > -\zeta$, they are equal for $\mu = (\zeta - \sqrt{2}E_b)/(\sqrt{2} - 1)$. In the normal state, the chemical potential of at least one of the spin components (up or down) should be positive for there to be any particles at all. This means that $\mu + \zeta > 0$ or $\mu - \zeta > 0$. For $\zeta > 0$, the first condition is easier to fulfill, so that it determines the boundary in the phase diagram with the "empty phase" (no particles).

Figure 1 shows the phase diagram of the superfluid (SF), normal (N), fully polarized normal (NP) and empty phases as a function of μ/E_b and ζ/E_b. This phase diagram looks qualitatively similar to the one obtained in 3D by mean field theory in Ref. [21].

Within this local density approximation, moving from the center of the trap towards the edge corresponds to moving down along the arrow in figure 1. From the center to the edge

we encounter first the balanced superfluid (SF), then a shell of spin-imbalanced normal gas, and finally a shell of fully polarized normal gas, as illustrated in the inset. The superfluid state in this treatment is balanced in the limit of temperature zero, but allows for imbalance for any $T > 0$.

In a typical experiment with a 1D optical lattice, several hundreds of layers are present. As long as the Fermi energy and the superfluid gap are much larger than the tunneling rate between the layers, the pairing is essentially a phenomenon that takes place within each layer individually [22] and each layer can be treated in the local density approximation by setting $\mu_0^{(i)} = \mu_0 - U^{(i)}$, where $U^{(i)}$ is the trapping potential at the center of the ith layer. The tunneling between the different layers is between layers of zero imbalance, so that the results of Refs. [17, 23] can be used.

The preceding saddle point calculation implicitly makes the mean field assumption that the typical size of the paired state ℓ_Δ is much larger than the distance between the fermionic atoms ℓ. Deep in the BEC limit, the system is in fact more suitably described as a Bose-Fermi mixture of strongly bound bosonic pairs and excess majority component atoms. We again can treat the 2D Bose-Fermi mixtures in the μ-ζ plane analytically. The energy density of the Bose-Fermi mixture is given by $E = 2\pi n_F^2 + g_{BB} n_B^2/2 + g_{BF} n_B n_F$ where the density of bosonic molecules n_B and of fermionic atoms n_F are positive. The coupling constant g_{BB} for dimer-dimer scattering in 2D has been calculated by Petrov et al. [24], but not that for dimer-atom scattering, g_{BF}. However in the limit of very low energy scattering, dimensional arguments show that to first order the dimer-dimer and dimer-atom scattering amplitudes are equal. The chemical potentials are $\mu_F = 4\pi n_F + g_{BF} n_B$ for the fermionic atoms and $\mu_B = g_{BB} n_B + g_{BF} n_F$ for the bosonic molecules.

A minimal energy state has a positive curvature as a function of the densities, i.e. the eigenvalues of $H_{ij} = \partial^2 E/\partial n_i \partial n_j$ have to be positive. A necessary condition is that its determinant is positive: $4\pi g_{BB} - g_{BF}^2 > 0$. Inverting the expressions for the chemical potential gives

$$n_F = \frac{g_{BB}\mu_F - g_{BF}\mu_B}{4\pi g_{BB} - g_{BF}^2} \tag{10}$$

$$n_B = \frac{4\pi\mu_B - g_{BF}\mu_F}{4\pi g_{BB} - g_{BF}^2} \tag{11}$$

The expressions (10), (11) provide us with the information on the phase diagram for phase separation of the 2D Bose-Fermi mixture. The condition for a finite number of fermions is

$\mu_F > g_{BF}\mu_B/g_{BB}$ and for a finite number of bosons, it is $\mu_B > g_{BF}\mu_F/4\pi$, where we have used $4\pi g_{BB} > g_{BF}^2$, as required for the stability of the system. To use the above results for the BEC side of the BEC/BCS crossover with imbalance, we substitute the bosonic chemical potential by $\mu_B \to \mu_\uparrow + \mu_\downarrow + E_b = 2\mu + E_b$ and the fermionic chemical potential by $\mu_F \to \mu_\uparrow = \mu + \zeta$. The condition for a finite molecule density is then

$$\mu > -\frac{E_b}{2}\left(1 - \frac{g_{BF}}{2\pi}\right) + \frac{g_{BF}}{4\pi}\zeta \tag{12}$$

while the condition for a finite fermion density reads

$$\mu < \frac{\zeta - E_b g_{BF}/g_{BB}}{2g_{BF}/g_{BB} - 1} \tag{13}$$

In between these limits, a mixture of bosonic molecules and fermionic atoms may coexist. Thus, we expect corrections beyond mean field to allow for an additional phase to appear in the phase diagram of Fig.1: the imbalanced superfluid, qualitatively indicated by the shaded region. Moreover, Eq. (13) indicates that the line separating the spin-balanced superfluid (molecules only) from the imbalanced superfluid lies below the mean field SF-NP phase boundary of Fig.1.

In conclusion, the experimental and theoretical investigation of resonance superfluidity in Fermi gases has been marked by two recent advances: the creation of a Fermi superfluid from a gas with unequal spin populations [5, 6], and the detection of fermionic superfluidity in an optical lattice [14]. We have combined both effects and studied the effect of unequal spin populations on the superfluidity in an optical lattice.

We derived an analytical expression for the free energy of the imbalanced 2D Fermi gas, eq. (6). From this result, the BEC/BCS gap equation and saddle-point number equations can be solved analytically, and results are provided for fixed imbalance δn in table (I) However, analyzing the free energy as a function of the superfluid gap we found that phase separation occurs, and a (possibly imbalanced) normal and (always balanced) superfluid phase separate. The phase boundaries are evaluated analytically. The shell structure of the inhomogeneously trapped gas is revealed to successively be from the center to the edges a balanced superfluid, the spin-imbalanced normal state and the fully polarized normal state. In the deep BEC limit a Bose-Fermi mixture offers a more suitable description than the mean-field picture. In this Bose-Fermi mixture, an imbalanced superfluid mixture of bosonic molecules and fermionic atoms is possible in addition to the phases identified earlier.

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